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INTEGRABLE Z_n -CHIRAL POTTS MODEL: THE MISSING RAPIDITY-MOMENTUM RELATION

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The McCoy-Roan integral representation for gaps of the integrable Z_n -symmetric Chiral Potts quantum chain is used to calculate the boundary of the incommensurate phase for various n . In the limit $n \rightarrow \infty$ an analytic formula for this phase boundary is obtained. The McCoy-Roan formula gives the gaps in terms of a rapidity. For the lowest gap we conjecture the relation of this rapidity to the physical momentum in the high-temperature limit using symmetry properties and comparing the McCoy-Roan formula to high-temperature expansions and finite-size data.

1 Introduction: Z_n -symmetrical Chiral Potts Quantum Chains

The Chiral Potts model has been introduced in 1981 by Ostlund¹ in order to describe commensurate-incommensurate (C-IC) phase transitions observed in surface monolayer adsorbates, e.g. krypton on a graphite surface. The location of a possible Lifshitz point in the phase diagram was a major issue. The quantum chain version has been used first by Centen *et al.*². After the discovery of the novel integrability properties of the Chiral Potts models^{3,4}, much interest has focussed on their mathematical aspects. Nevertheless, the spectrum of the Chiral Potts quantum chains exhibits several unusual interesting physical features caused by the inherent parity violation.

The Z_n -symmetrical Chiral Potts quantum chains are defined by

$$H^{(n)} = - \sum_{i=1}^N \sum_{k=1}^{n-1} \left\{ \bar{\alpha}_k \sigma_i^k + \lambda \alpha_k \Gamma_i^k \Gamma_{i+1}^{n-k} \right\}. \quad (1)$$

The operators σ_i and Γ_i act in a vector space C^n located at site i and satisfy

$$\sigma_i \Gamma_j = \Gamma_j \sigma_i \omega^{\delta_{i,j}}; \quad \sigma_i^n = \Gamma_i^n = 1; \quad \sigma_i^+ = \sigma_i^{n-1}; \quad \Gamma_i^+ = \Gamma_i^{n-1} \quad (2)$$

where $\omega = e^{2\pi i/n}$. The parameter $\lambda \geq 0$ plays the rôle of an inverse temperature (we shall consider the ferromagnetic case only). $\bar{\alpha}_k$ and α_k are complex parameters. If we choose to represent the σ_i by diagonal matrices $(\sigma_i)_{l,m} = \omega^{l-1} \delta_{l,m}$ then the Γ_i become cyclic lowering operators $(\Gamma_i)_{l,m} = \delta_{l,m+1}$. N is the number of sites. We use periodic boundary conditions $\Gamma_{N+1} = \Gamma_1$.

A three-parameter version of (1), expressing the coefficients in terms of just two chiral angles $0 \leq \varphi, \phi \leq \pi$:

$$\bar{\alpha}_k = e^{i\varphi(\frac{2k}{n}-1)} / \sin(\pi k/n); \quad \alpha_k = e^{i\phi(\frac{2k}{n}-1)} / \sin(\pi k/n) \quad (3)$$

describes various cases of particular interest:

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- For general n and $\varphi = \phi = 0$ we recover the Fateev-Zamolodchikov parafermionic model, for $n=2$ we get the standard Ising quantum chain.
- If $\varphi = \phi = \pi/2$ we get a representation of the Onsager-Dolan-Grady-algebra : "Superintegrable Chiral Potts-Model" ^{3,5}.
- Au-Yang *et al.* ⁴ have shown that (1),(3) can be derived from a two-dimensional lattice model with (generally complex) Boltzmann weights satisfying Yang-Baxter equations (so that $H^{(n)}$ is integrable) if the three parameters are related by

$$\cos \varphi = \lambda \cos \phi. \quad (4)$$

- Eq.(4) forces $H^{(n)}$ to become non-hermitian⁶ for $\lambda < 1$ if we choose $|\cos \varphi| > \lambda$. For (4) with $\cos \varphi > \lambda$ the hamiltonian is parity invariant up to complex conjugation, whereas for (4) with $\cos \varphi < -\lambda$ there is a more complicated shifted parity symmetry^{7,8}, see eq.(15) below.

$H^{(n)}$ is Z_n -symmetrical and translational invariant. So, its spectrum decomposes into sectors labeled by the Z_n -charge $Q = 0, \dots, n-1$ and P , the momentum eigenvalue which takes the values $0 \leq P = 2\pi k/N < 2\pi$ with $k = 0, 1, \dots, N-1$ or $-[N/2] < k \leq [N/2]$.

We denote the eigenvalues of $H^{(n)}$ at fixed λ, φ (in this talk ϕ will always be determined by (4)) by $E_{Q,r}(P)$. The index $r = 0, 1, \dots$ labels the levels in each Q, P -sector, starting with $r = 0$ as the ground-state of the respective sector. In some part, but not in all regions of the λ, φ -plane, the ground state of H is in the $Q = P = 0$ -sector. By convention, we shall define gaps *always* with respect to the lowest $Q = P = 0$ -level at the same λ, ϕ and φ :

$$\Delta E_{Q,r}(P) =: E_{Q,r}(P) - E_{0,0}(P = 0). \quad (5)$$

Since in general parity is not conserved, a relation $E(P, \lambda, \varphi) = E(-P, \lambda, \varphi)$ is expected to be valid only for special values of λ and φ . Consequently, in general the minimum of $E(P, \lambda, \varphi)$ is not at $P = 0$ as is seen e.g. in Fig. 2. Quite generally, the spectrum of $H^{(n)}$ seems to be a quasiparticle spectrum^{9,10,11} with one quasiparticle in each $Q \neq 0$ -charge sector and one or more exceptional "Cooper-excitations"⁹. In the IC phase the ground state loses translational invariance, because there the $Q = 1$ -quasiparticle dispersion curve dips below the lowest $Q = P = 0$ -level for a certain range of $P \neq 0$ and $\Delta E_{Q=1,r=0}(P)$ becomes negative.

2 The McCoy-Roan gap formula

While for the Z_3 -superintegrable case the complete spectrum of $H^{(n)}$ has been calculated analytically^{7,9}, only few details are known about the spectrum in the more general integrable case (4). In the rest of this talk, we shall consider this integrable case. The difficulty of making progress here comes because in this case the rapidity parameters appearing in the Yang-Baxter-equations are restricted to higher elliptic curves. Baxter¹² has devised an approach which avoids uniformization of the spectral variables. Solving a functional equation⁷ due to Baxter, Bazhanov and Perk¹⁴, McCoy and Roan for Z_3 , and then McCoy for the general Z_n -case¹³ have derived an analytic formula for the

low-temperature gap in the thermodynamic limit. By duality, this is equivalent to the following expression for the lowest $\Delta Q = 1$ gap in the high-temperature regime $\lambda < 1$:

$$\begin{aligned} \Delta E_{1,0}(\bar{v}) = & 2(1 - \lambda)\bar{t}_p^{n/2} \pm 2\bar{v}\bar{t}_p^{-\frac{n}{2}+1} \frac{\sqrt{(\bar{t}_p^n - 1) \{(1 + \lambda)^2 - (1 - \lambda)^2 \bar{t}_p^n\}}}{(\omega^{1/2}\bar{v}\bar{t}_p - 1)(\omega^{-1/2}\bar{v}\bar{t}_p - 1)} \sin \frac{\pi}{n} \\ & + n\bar{v}\bar{t}_p^{n/2} \frac{\mathcal{P}}{\pi} \int_1^{(\frac{1+\lambda}{1-\lambda})^{2/n}} d\bar{t} \frac{2(\bar{t}\bar{v} - \cos \frac{\pi}{n})}{(\bar{t}\bar{v})^2 - 2\bar{t}\bar{v} \cos \frac{\pi}{n} - 1} \frac{\sqrt{(\bar{t}^n - 1) \{(1 + \lambda)^2 - (1 - \lambda)^2 \bar{t}^n\}}}{\bar{t}^n - \bar{t}_p^n} \end{aligned} \quad (6)$$

Here \mathcal{P} in front of the integral indicates the principal value. The sign \pm in front of the second term has to be chosen "+" for $0 \leq \phi < \frac{\pi}{2}$ and "-" for $\frac{\pi}{2} < \phi \leq \pi$. The chiral angle ϕ enters (6) only in the combination

$$f(\lambda, \phi) = 1 - 2\lambda \cos(\phi - \varphi) + \lambda^2 \quad (7)$$

through $\bar{t}_p^n = f(\lambda, \phi)/(1 - \lambda)^2$. \bar{v} is a rapidity parameter which will also be used in the form $v = ((1 + \lambda)/(1 - \lambda))^{1/n} \bar{v}$. The relation of v or \bar{v} to the physical momentum P will be our main concern. Only in the Z_3 superintegrable case it is known⁷ to read $\exp(-iP) = (1 + \omega^2 \bar{v})/(1 + \omega \bar{v})$.

We find it useful to recast (6) into the following form:

$$\begin{aligned} \Delta E_{1,0}(v, \lambda) = & 2\sqrt{f(\lambda, \phi)} \left\{ 1 + 2 \Im m \frac{1}{1 - \nu_p^{-1} \omega^{1/2}} \Im m \frac{1}{1 - \lambda e^{-i(\phi - \varphi)}} \right. \\ & \left. + \frac{1}{\pi} \mathcal{P} \int_{-1}^1 \frac{dx}{\cos(\phi - \varphi) - x} 2 \Re e \frac{1}{1 - \nu^{-1} \omega^{1/2}} \Im m \frac{1}{1 - \lambda e^{i \arccos x}} \right\} \end{aligned} \quad (8)$$

where

$$\nu = \left(\frac{1 - 2\lambda x + \lambda^2}{1 - \lambda^2} \right)^{\frac{1}{n}} v \quad \text{and} \quad \nu_p = \left(\frac{f(\lambda, \phi)}{1 - \lambda^2} \right)^{\frac{1}{n}} v. \quad (9)$$

The form (8) has the advantage that now v appears only in two places via ν_p and ν . In the superintegrable case one has $\phi = \varphi$ so that $\bar{t}_p = 1$ and in (8) the second term of the curly bracket vanishes. Recall that on the boundary of the hermitian region $\phi = 0$ or $\phi = \pi$ so that $\cos \varphi = \pm \lambda$ and we have $\cos(\phi - \varphi) = \lambda$ and $\bar{t}_p = ((1 + \lambda)/(1 - \lambda))^{1/n}$.

From (8) we see that for $v = 0, \infty$ the n -dependence (which is due only to the factors $\omega^{1/2}$, ν and ν_p) disappears. For $v = 0$ we get immediately

$$\Delta E_{1,0}(v = 0, \lambda) = 2\sqrt{f(\lambda, \phi)} = \begin{cases} 2\sqrt{1 - \lambda^2} & : \phi = 0, \pi \\ 2(1 - \lambda) & : \phi = \frac{\pi}{2} \end{cases}, \quad (10)$$

while for $v = \infty$ the principal value integral can be calculated analytically, leading to

$$\Delta E_{1,0}(v = \infty, \lambda) = \frac{2(1 - \lambda^2)}{\sqrt{f(\lambda, \phi)}} = \begin{cases} 2\sqrt{1 - \lambda^2} & : \phi = 0, \pi \\ 2(1 + \lambda) & : \phi = \frac{\pi}{2} \end{cases}. \quad (11)$$

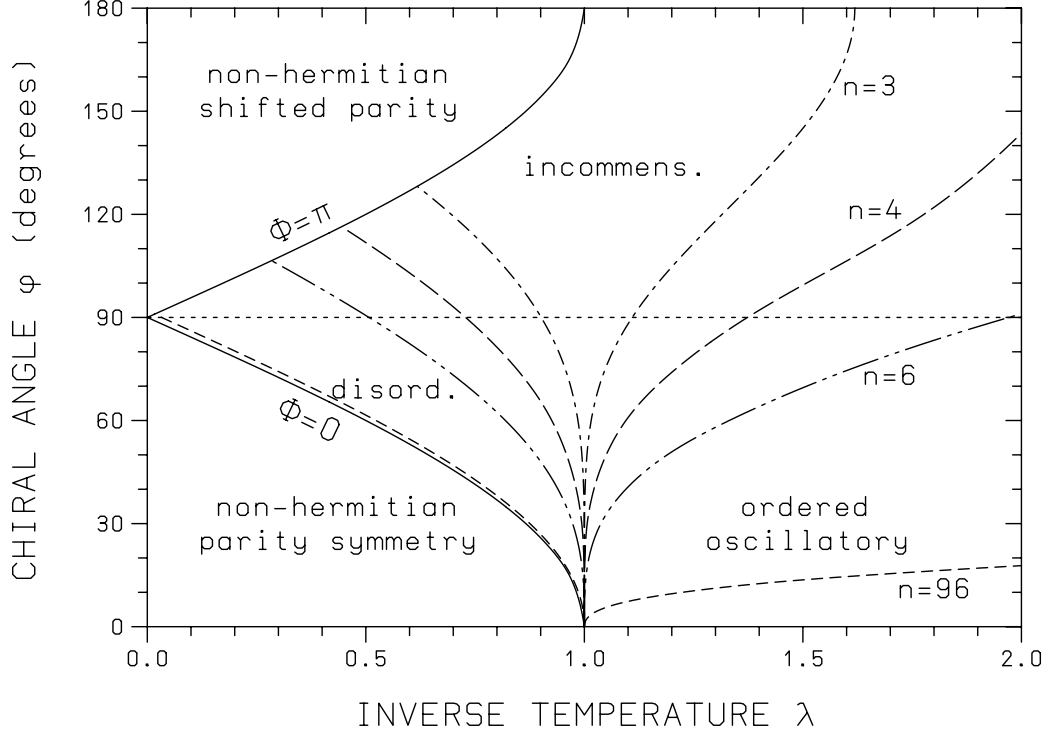


Figure 1: Phase diagram of the integrable Chiral Potts model showing the boundaries of the non-hermitian region $\phi = 0, \pi$ (full curves). The dashed-dotted curves give the boundaries of the IC phase for the Z_n -models with $n = 3, 4, 6, 96$.

3 Boundary of the region where $\Delta E_{Q=1}$ becomes negative.

As was already mentioned at the end of Sec.1, the C-IC phase transition arises where the ground state loses translational invariance. This is the case where $\Delta E_{Q=1}(P)$, by varying λ at fixed φ , as a function of P acquires a second order zero at some $P \neq 0$.

In the regime where parity-invariance is broken, in general the second order zero will appear at $P \neq 0$ anyway. Therefore, even not knowing the precise relation between v and P , we can as well look in (6) or (8) for such a second order zero as a function of v . In ref.¹³ McCoy and Roan have used this method to obtain the IC phase boundary for Z_3 . For general Z_n , since the analogue of the McCoy-Roan formula for gaps with $Q \geq 2$ has not been worked out, there are only qualitative arguments (experience from finite-size calculations) that it is the $Q = 1$ -gap and not a higher- Q gap which determines the C-IC phase boundary.

For the $\Delta E_{Q=1}$ -gap we did the calculation for many values of n for various φ and obtain the curves shown in Fig. 1. The low- and high-temperature IC-phase boundaries are related by duality: $\lambda \leftrightarrow \lambda^{-1}$ together with $\varphi \leftrightarrow \phi$.

Looking at our numerical results for very large n ($n = 10^3 \dots 10^5$) we found that in the limit $\sqrt{n} \sin(\varphi/2) \rightarrow \infty$ the phase boundary curve $\lambda_c(\varphi)$ and the corresponding value of v at the second order zero, v_c , assume the simple form (here we give the values λ_c for the low-temperature branch):

$$\lambda_c = \frac{2n}{\pi} \sin^2(\varphi/2) + \dots; \quad v_c = 1 - \frac{\pi}{n} \cot(\varphi/2) + \dots \quad (12)$$

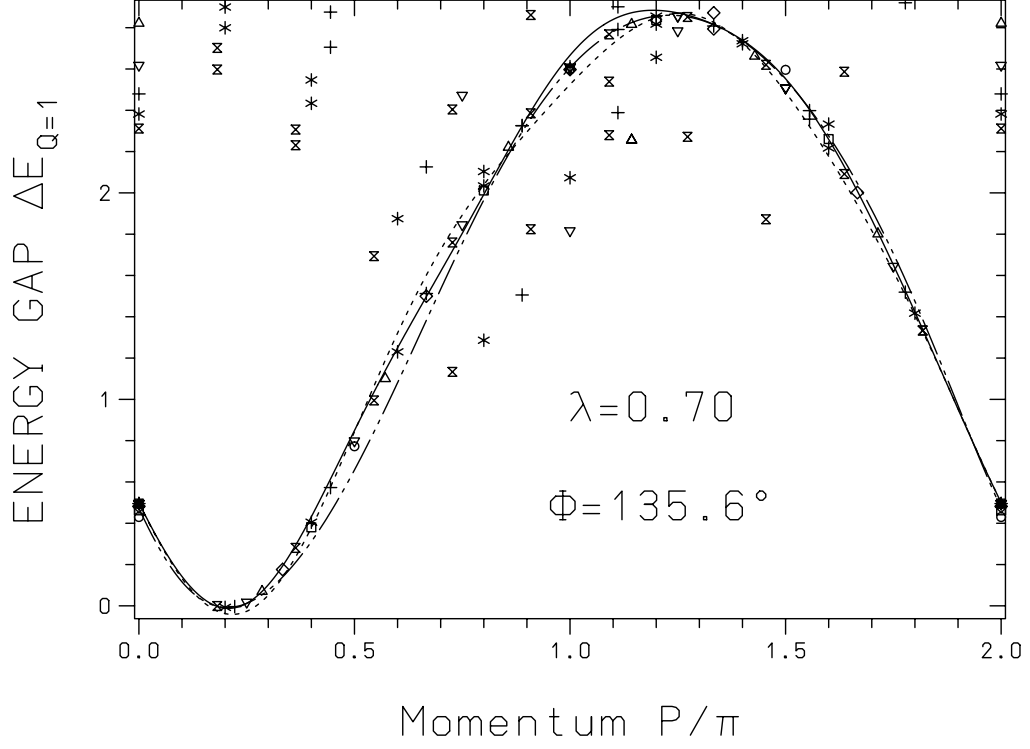


Figure 2: Energy-momentum plot of low-lying levels in the $Q = 1$ -sector of the Z_3 -integrable Chiral Potts model for $\lambda = 0.7$ and $\varphi = 120^\circ$ (which is close to the C-IC-phase boundary since $\Delta E_{Q=1}$ is just getting negative at $P \approx 0.2\pi$). Dashed-dots curve: McCoy-Roan formula using our rapidity-momentum relation (16). Full and dotted curves: expansion to 4th and 3rd order in λ , respectively. Symbols: finite-size data for up to $N = 11$ sites.

For $\varphi \ll 1$ the IC phase forms a wedge around $\lambda = 1$ described by $\lambda_c - 1 = a_n \varphi^{2n/(n-2)} + \dots$ where $a_3 = 0.0185(2)$; $a_4 = 0.0883(3)$; $a_5 = 0.153(1)$; $a_6 = 0.204(2)$. Notice that for small n this is very narrow.

Once knowing the result (12) it is not difficult to prove it analytically from (8) expanding λ_c^{-1} and $v_c - 1$ in powers of $q = \pi/n$. Recall that the n -dependence comes in (8) only through $\omega^{1/2}$, ν and ν_p . Two principal value integrals appear, which can be calculated explicitly.

4 Determination of the Rapidity-Momentum Relation

In view of the difficulties with high genus Riemann surfaces, probably it will take some time until someone will come up with an analytic derivation of the dependence $P(v)$ for the gap $\Delta E_{Q=1}$ at general n , λ and φ . Therefore we find it worthwhile to do what is possible right away, which is to combine numerical and symmetry information for deducing the main behaviour of $P(v)$:

1) Numerical diagonalization of $H^{(n)}$ for up to $N = 3 \dots 12$ sites is easy and leads to a quite precise determination of the gap $\Delta E_{Q=1, r=0}(P)$ over most part of the region $0 \leq \lambda \leq 0.9$ and $0 \leq \varphi < 120^\circ$. A third order high-temperature expansion (which we performed up to $n = 8$) leads to almost the same values even up to $\lambda \approx 0.7$, only at

larger λ there are problems for $P \leq \frac{\pi}{2}$, see the Figures for Z_3 given in ref. ¹¹.

All these results show that $\Delta E_{Q=1,r=0}(P)$ is smooth with just one maximum and one minimum in the first Brillouin zone of P . Also (8) for fixed n , λ , φ as a function of v has only one single maximum and minimum in the whole range $-\infty < v < +\infty$. Therefore numerically it is easy to determine the mapping $P(v)$ which brings both curves into coincidence.

2) Applying this method to the superintegrable line, after some educated guesswork we find that the Z_3 formula quoted in the text before eq.(9), should be generalized to Z_n as:

$$e^{-iP} = \frac{1 - \omega^{1/2}\bar{v}}{1 - \omega^{-1/2}\bar{v}} \quad \text{or} \quad \bar{v} = -\frac{\sin \frac{1}{2}P}{\sin \frac{1}{2}(P - P_\infty)} \quad \text{with} \quad P_\infty = \frac{2\pi(n-1)}{n}. \quad (13)$$

3) We want to summarize also other numerical results in a compact empirical formula (which for $\varphi \rightarrow \frac{\pi}{2}$ has to reduce to (13)). For this purpose we use the fact that at the boundaries of the hermitian region $\phi = 0, \pi$ there are special reflection symmetries ⁸, which follow from eq.(B.18) of Albertini *et al.*⁷, and which determine $P(v)$ at $v = \pm 1$:

- At the lower boundary $\phi = 0$ (see Fig.1) $H^{(n)}$ is parity invariant. In (8) this feature shows up as symmetry ^b under $v \leftrightarrow v^{-1}$ which appears just at $\phi = 0$. So at $\phi = 0$, comparing also the numerical data, for $0 \leq \lambda < 1$ we get

$$P(v) = 2\pi - P(v^{-1}); \quad \text{so that} \quad P(v = 1) = \pi; \quad P(v = -1) = 0. \quad (14)$$

- For $\phi = \pi$ the spectra have a charge-sector-dependent shifted parity symmetry ^{7,8}, which again corresponds to a symmetry of (8) against $v \leftrightarrow v^{-1}$. Using (B.18) of ref. ⁷ we find at $\phi = \pi$ for $0 \leq \lambda < 1$

$$\begin{aligned} P(v) &= 2\pi - P(v^{-1}) - 4\pi/n \\ \text{so that} \quad P(v = 1) &= (n-2)\pi/n; \quad P(v = -1) = 2(n-1)\pi/n. \end{aligned} \quad (15)$$

By making the following ansatz for ν_p (ν_p is proportional to v , see (9)), we fulfil all constraints (14), (15) and for $\varphi = \phi = \frac{\pi}{2}$ obtain (13):

$$\nu_p = -\frac{\sin \frac{1}{2}(P - P_0)}{\sin \frac{1}{2}(P - P_\infty)} \quad \text{with} \quad P_0 = -2(\phi - \varphi)/n; \quad P_\infty = 2\pi - 2(\phi + \varphi)/n. \quad (16)$$

We have calculated various dispersion curves using (8) with (16) and compared these to finite-size- and perturbative data for the Z_3 to Z_7 -models. Because of space limitations, we show only Fig. 2 which gives a non-trivial example. For $0 \leq \lambda < 0.4$ the agreement is so good that we conjecture (16) to be exact in the limit $\lambda \rightarrow 0$. A disagreement arises if we move towards the parafermionic corner $\lambda \rightarrow 1$, $\phi \rightarrow 0$. Here the momentum interval corresponding to positive v expands such that finally there is only a small interval around $P = 2\pi$ left for the whole negative region $-\infty < v < 0$. Put differently, both P_∞ and P_0 seem to converge to $P = 0$ as we move towards $\lambda = 1$ on the curve $\phi = 0$. The ansatz (16) does not yet take care of this behaviour. For the Z_3 -case and $0.95 < \lambda < 0.999$, $\phi = 0$ a good fit can be obtained neglecting the negative v -region altogether using $v = |\tan \frac{P}{4}|^{2/3}$. There $\Delta E_{Q=1,r=0}(P)$ becomes λ -independent with a peak value of $\Delta E_{Q=1} = 6$ at $P = \pi$ or $v = 1$.

^bObserve that the symmetry is in v and *not* in \bar{v}

5 Conclusions

Comparing the McCoy-Roan formula for the lowest gap of the integrable Z_n -Chiral Potts model to finite-size and perturbative data and using the special symmetry properties at the boundary of the hermitian regime, we obtain information about the hitherto unknown relation between the rapidity parameter and the physical momentum *off* the superintegrable line. The numerical agreement suggests that the conjectured formula (16) may be exact in the high-temperature limit. We also find an analytic formula for the IC-phase boundary curve of the integrable Z_n -Chiral Potts model valid for large $\sqrt{n} \sin(\varphi/2)$. For $n \rightarrow \infty$ the whole superintegrable line will be in the IC-phase.

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